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The maximum Randić index of chemical trees with k pendants[☆]

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ABSTRACT

A tree is a chemical tree if its maximum degree is at most 4. Hansen and Mélot [P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs 6: analyzing bounds for the connectivity index, J. Chem. Inf. Comput. Sci. 43 (2003) 1–14], Li and Shi [X. Li, Y.T. Shi, Corrections of proofs for Hansen and Mélot's two theorems, Discrete Appl. Math., 155 (2007) 2365–2370] investigated extremal Randić indices of the chemical trees of order n with k pendants. In their papers, they obtained that an upper bound for Randić index is $\frac{n}{2}+\frac{(3\sqrt{2}+\sqrt{6}-7)k}{6}$. This upper bound is sharp for $n \geq 3k-2$ but not for $n < 3k-2$. In this paper, we find the maximum Randić index for $n < 3k-2$. Examples of chemical trees corresponding to the maximum Randić indices are also constructed.

1. Introduction

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies (see [4,5,11]). Among the numerous topological indices considered in chemical graph theory, only a few have been found to be noteworthy in practical application (see [9]). One of these is Randić index. Randić index (also called connectivity index) of an organic molecule whose molecular graph is $G=(V,E)$ is defined (see [2,10]) as

$$R(G)=\sum_{uv\in E}(d(u)d(v))^{-\frac{1}{2}},$$

where $d(u)$ denotes the degree of the vertex u of G. In Randić's study of alkanes, he showed that if alkanes are ordered in the descending order according to the $R(G)$-values, then the extent of their branching should increase (see [1]). There are many works on studying trees with extremal Randić index, which can be found in the monograph [6] written by Gutman and Li.

For any tree T, we denote
$V_i(T)=\{v\in V(T):d_T(v)=i\}$, $n_i(T)=|V_i(T)|$.
$N(V')=\{v\in V(T):u\in V', uv\in E(T)\}\setminus V'$ for $V'\subset V(T)$.
$E_{ij}(T)=\{uv\in E(T):d_T(u)=i, d_T(v)=j\}$, $e_{ij}(T)=|E_{ij}(T)|$.
Randić index of a tree T with maximum degree Δ can be expressed as

$$R(T)=\sum_{1\le i\le j\le \Delta}\frac{e_{ij}(T)}{\sqrt{i\times j}}. \tag{1.1}$$

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For simpleness, we often write V_i, $N(V_i)$, n_i and e_{ij} instead of $V_i(T)$, $N(V_i(T))$, $n_i(T)$ and $e_{ij}(T)$, $1 \le i \le j \le \Delta$, respectively if there is no ambiguity.

A *chemical tree* is a tree whose maximum degree is at most 4. The extremal Randić indices of trees of order n with k pendants are investigated in [8,12,13]. Hansen and Mélot [3], Li and Shi [7] investigated extremal Randić indices of the chemical trees of order n with k pendants. In their papers, they obtained that an upper bound for Randić index is $\frac{n}{2} + \frac{(3\sqrt{2}+\sqrt{6}-7)k}{6}$. This upper bound is tight for a specific class of trees constructed by Hansen and Mélot [3]. However, such trees exist only when $n \ge 3k-2$. For $n < 3k-2$, this upper bound is not tight.

It is clear that the order of a tree with k pendants is at least $(3k-2)/2$. The main purpose of this paper is to determine the maximum Randić index and their structures of the chemical trees of order n with k pendants for $n < 3k-2$.

In the following sections, we first characterize some properties of chemical trees attained the maximum Randić index, and then describe some formulas to calculate the number of n_i and e_{st}, where $2 \le i \le 4$, $1 \le s \le t \le 4$, and $t \ne 1$. Finally, we determine the maximum Randić indices and structures of the chemical trees of order n with k pendants for $n < 3k-2$.

2. Properties of maximal chemical trees

Suppose T is a tree. A path P in T is called an *i-degree pendant chain* if all of its internal vertices are of degree 2 and its ends of degree 1 and i respectively, where $i \ge 3$. In particular, P is called an *i-degree pendant edge* if P is an edge. Now we only consider chemical trees here.

For convenience, denote that $\mathcal{T}_{n,k} = \{T : T \text{ is a chemical tree of order } n \text{ with } k \text{ pendants}\}$ and $R_{\max}(\mathcal{T}_{n,k}) = \max\{R(T) : T \in \mathcal{T}_{n,k}\}$. A chemical tree $T \in \mathcal{T}_{n,k}$ with $R(T) = R_{\max}(\mathcal{T}_{n,k})$ is called a *maximal chemical tree*.

Lemma 2.1 ([12]). *Vertices with degree 2 of a maximal chemical tree lie on pendant chains.*

Lemma 2.2 ([12]). *Suppose T is a maximal chemical tree. If P is a path in T with ends of degree 4, then all internal vertices of P are of degree 4.*

For any chemical tree $T \in \mathcal{T}_{n,k}$, we have

$$\begin{cases} n = k + n_2 + n_3 + n_4 \\ k = n_3 + 2n_4 + 2 \\ k = n_1 = e_{12} + e_{13} + e_{14}. \end{cases} \tag{2.1}$$

Lemmas 2.1 and 2.2 imply that if T is a maximal chemical tree, then the subgraphs $T - (V_1 \cup V_2)$ and $T - (V_1 \cup V_2 \cup V_3)$ of T are trees (if they are not empty sets), respectively. Since $|V(T - (V_1 \cup V_2))| = |E(T - (V_1 \cup V_2))| + 1$ and $|V(T - (V_1 \cup V_2 \cup V_3))| = |E(T - (V_1 \cup V_2 \cup V_3))| + 1$, we have if $n_4 = 0$ and $n_3 \ne 0$, then $e_{33} = n_3 - 1$, and if $n_4 \ne 0$, then $e_{44} = n_4 - 1$. Moreover there exist bijections between vertex set V_2 and edge set $E_{22} \cup E_{23} \cup E_{24}$ if $n_3 + n_4 \ne 0$, vertex set V_3 and edge set $E_{33} \cup E_{34}$ if $n_4 \ne 0$, respectively. Thus we have $n_2 = e_{22} + e_{23} + e_{24}$ and $n_3 = e_{34} + e_{33}$. By Lemma 2.1, there is a bijection between V_2 and $E_{12} \cup E_{22}$. Hence we have $n_2 = e_{12} + e_{22}$. The results above are summarized as follows:

Corollary 2.3. *For any maximal chemical tree T, we have*

(1) *if* $n_4 = 0$ *and* $n_3 \ne 0$, *then* $n_3 = e_{33} + 1$;
(2) *if* $n_4 \ne 0$, *then* $n_4 = e_{44} + 1$;
(3) *if* $n_3 + n_4 \ne 0$, *then* $n_2 = e_{22} + e_{23} + e_{24}$;
(4) *if* $n_4 \ne 0$, *then* $n_3 = e_{34} + e_{33}$;
(5) $n_2 = e_{12} + e_{22}$.

Note that if $n_4 \ne 0$, then the induced subgraph of vertex set $V_4 \cup N(V_4)$ is also a tree with the pendant vertex set $N(V_4)$. By the second formula in (2.1), $|N(V_4)| = 2n_4 + 2$. On the other hand $|N(V_4)| = e_{14} + e_{24} + e_{34}$. Combining Corollary 2.3(4), we have the following corollary.

Corollary 2.4. *Suppose T is a maximal chemical tree. If $n_4 \ne 0$, then*

(1) $2n_4 + 2 = e_{14} + e_{24} + e_{34}$;
(2) $n_3 - (2n_4 + 2) = e_{33} - e_{14} - e_{24}$.

Lemma 2.5 ([12]). *For any maximal chemical tree T, we have*

(1) $e_{24} < 4$;
(2) *either* $e_{14} = 0$ *or* $n_2 = 0$;
(3) *either* $e_{14} = e_{24} = 0$ *or* $e_{33} = 0$;
(4) *either* $e_{22} = 0$ *or* $n_4 = e_{13} = 0$.

Throughout this paper, we shall use $T[E_{33}]$ to denote the subgraph of T induced by $E_{33}(T)$ for any tree T.

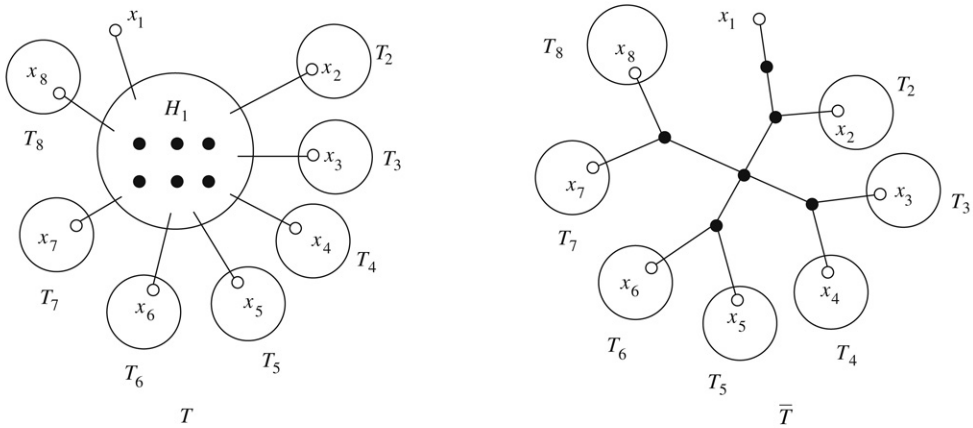

Fig. 1. Figure for the proof of Lemma 2.6(1).

Lemma 2.6. *Suppose T is a maximal chemical tree. Then we have*

(1) *if $e_{13} \neq 0$, then $e_{33} \leq 4$,*
(2) *if $n_4 \neq 0$ and $e_{13} \neq 0$, then $e_{23} + e_{33} < 3$.*

Proof. Note the fact that if $v_0v_1 \cdots v_{k-1}v_k (k \geq 1)$ is a path in a tree T with $d_T(v_0) = d_T(v_k) \geq 2$, $u \in N_T(v_0) \setminus \{v_1\}$ and $w \in N_T(v_k) \setminus \{v_{k-1}\}$ then $T' = T - \{v_0u, v_kw\} + \{v_0w, v_ku\}$ is still a tree. By the definition of Randić index, we have $R(T') = R(T)$. We may assume that $H = T[E_{33}]$ is connected. Otherwise, suppose there are two components H_1 and H_2 of H. Since there is an unique path between two vertices in T, we can assume that $uv_0 \in E(H_1)$, $v_{k-1}v_k \in E(H_2)$ and $v_0v_1 \notin E(H_1)$. By the transfer process described above, the new tree T' has a component of $T'[E_{3,3}]$ containing more edges than H_2. By repeating this process, we can get a tree such that its induced subgraph of E_{33} is connected and its Randić index is the same value as $R(T)$. Since $e_{13} \neq 0$, there is an edge $e = x_1u \in E_{13}$. By using the above transfer process we may assume that $u \in V(H)$. So we will assume that H is connected and x_1 is a pendant adjacent to one of vertices in H (or H_1) in the following proof.

Suppose $e_{33} \geq 5$. Then $|V(H)| \geq 6$. Let H_1 be a subtree of H and $|V(H_1)| = 6$. Since H_1 contains 5 edges, there are $\sum_{v \in V(H_1)} d_T(v) - 2|E(H_1)| = 3 \times 6 - 2 \times 5 = 8$ vertices in $N(V(H_1))$, say x_i, $1 \leq i \leq 8$ (x_1 is defined above). Let T_i be the subtree of T rooted at x_i for $1 \leq i \leq 8$ described in Fig. 1 (T_1 is the trivial tree consisting of x_1). Also vertices of H_1 are represented by solid vertices in Fig. 1. By using $T_1, \ldots, T_8$ we can construct a tree $\overline{T}$ which is obtained from T by rearranging those solid vertices as shown in the right-hand side of Fig. 1.

Then $\overline{T} \in \mathcal{T}_{n,k}$ and

$$R(\overline{T}) - R(T) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{12}} - \frac{1}{\sqrt{3}} - \frac{5}{3} > 0,$$

which contradicts to T being a maximal chemical tree in $\mathcal{T}_{n,k}$. So we have proved the first part of the lemma.

Next we prove the second part of the lemma by contradiction according to the following three cases respectively. Since $n_4 \neq 0$ and $e_{13} \geq 1$ we may assume that there are vertices $x_0, x_1 \in N(V(H))$ such that $x_0 \in V_4$ and $x_1 \in V_1$.

Case 1. If $e_{33} \geq 3$, then there are at least four vertices in $V(H)$. Let H_1 be a subtree of H with four vertices, by the argument of the paragraph above, there is a maximal chemical tree T, which is shown in the left-hand side of Fig. 2, where four solid vertices are in $V(H_1)$ with six neighbors $x_0, x_1, x_2, x_3, x_4, x_5$, and T_i is the subtree of T rooted at x_i for $0 \leq i \leq 5$. We can construct another tree $\overline{T}$ shown in the right-hand side of Fig. 2.

Thus we have

$$R(\overline{T}) - R(T) = \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{12}} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{16}} - \left(\frac{3}{\sqrt{9}} + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{3}}\right) > 0.$$

It contradicts to the choice of T.

Case 2. If $e_{33} = 2$ and $e_{23} \geq 1$, then $|V(H)| = 3$ and $d_T(x_i) \leq 2$ for $1 \leq i \leq 4$ (see Fig. 3).

Similar to Case 1 we have

$$R(\overline{T}) - R(T) = \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{8}} + \frac{1}{\sqrt{16}} - \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{9}}\right) > 0.$$

It yields a contradiction.

Case 3. If $e_{33} = 1$ and $e_{23} \geq 2$. Similar to Case 2, we have Fig. 4, where $d(x_2) = d(x_3) = 2$.

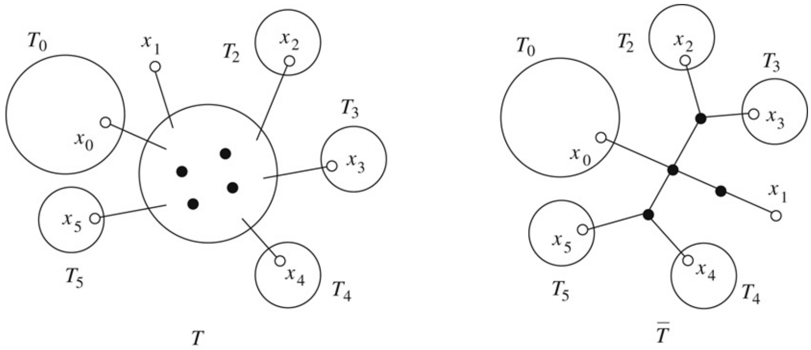

Fig. 2. Figures for the proof of Case 1.

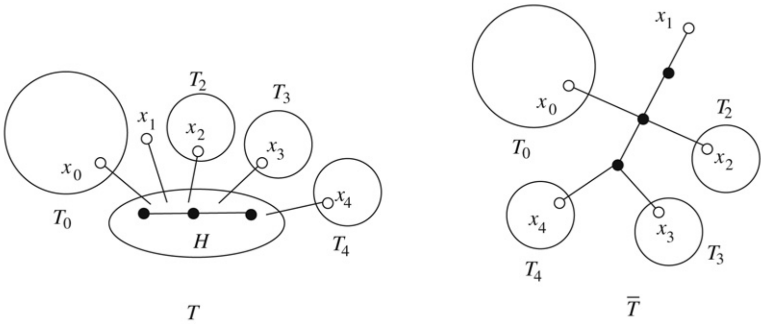

Fig. 3. Figures for the proof of Case 2.

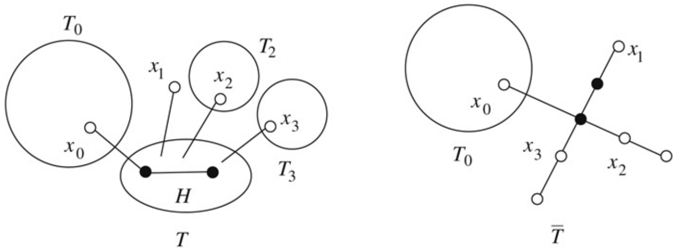

Fig. 4. Figures for the proof of Case 3.

Thus we have

$$R(\overline{T}) - R(T) = \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{8}} + \frac{1}{\sqrt{16}} - \left(\frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{9}} + \frac{1}{\sqrt{12}}\right) > 0.$$

It yields a contradiction. Therefore, we have the second part of the lemma. And the proof of the lemma is complete. □

Lemma 2.7. *Suppose $T \in \mathcal{T}_{n,k}$ is a maximal chemical tree. If $n < 3k - 2$ and $k \geq 8$, then $n_4 \neq 0$. Moreover, $e_{22} = 0$ and $n_2 = e_{12} < k$.*

Proof. If $n_4 = 0$, then $e_{14} = 0$. From the second and third formulas in (2.1) we have $n_3 = k - 2 > 0$ and $e_{13} = k - e_{12}$. By the first formula in (2.1) and $n < 3k - 2$ we have $k > n_2$. Hence we have $e_{13} = k - e_{12} \geq k - n_2 > 0$. By Lemma 2.6(1) we have $e_{33} \leq 4$. Since $n_4 = 0$ and $n_3 \neq 0$, by Corollary 2.3(1) we have $e_{33} = n_3 - 1 = k - 3 \geq 5$. It yields a contradiction. Therefore $n_4 \neq 0$.

Furthermore, by Lemma 2.5(4) and Corollary 2.3(5), we have $e_{22} = 0$ and $n_2 = e_{12} < k$. □

Corollary 2.8. *Suppose $T \in \mathcal{T}_{n,k}$ is a maximal chemical tree. For $n < 3k - 2$ and $k \geq 8$, if $n_3 \geq 2n_4 + 2$, then*

(1) $e_{14} = 0$, $e_{24} = 0$;
(2) $e_{13} = k - n_2$, $e_{23} = n_2$;
(3) $e_{33} = 2n_3 - k$, $e_{34} = k - n_3$.

Proof. By Lemma 2.7, we know that $n_4 \neq 0$ and $e_{22} = 0$. From Corollary 2.4(2) and $n_3 \geq 2n_4 + 2$, we have $e_{33} = e_{14} + e_{24} + n_3 - (2n_4 + 2) \geq e_{14} + e_{24}$. Since either $e_{14} = e_{24} = 0$ or $e_{33} = 0$ (Lemma 2.5(3)), we have $e_{14} = e_{24} = 0$. Hence we obtain (1).

Since $e_{22} = 0$ and $e_{24} = 0$ by (1), from Corollary 2.3(3) we have $e_{23} = n_2$. From the third formula of (2.1) we have $e_{13} = k - e_{12} - e_{14} = k - n_2$. Hence we obtain (2).

From (1) and the second formula of (2.1) we have $e_{14} = e_{24} = 0$ and $k = n_3 + 2n_4 + 2$. By Corollary 2.4 we have $e_{33} = n_3 - (2n_4 + 2) = 2n_3 - k$ and $e_{34} = 2n_4 + 2 = k - n_3$. Hence we get (3). □

3. The maximum Randić index of chemical tree

In this section, we first determine the numbers n_i, for $1 \leq i \leq 4$, of a maximal chemical tree, and then determine the numbers e_{ij}, for $1 \leq i \leq j \leq 4$. Finally, we determine Randić index of the tree.

Theorem 3.1. *Suppose $T \in \mathcal{T}_{n,k}$ is a maximal chemical tree with $n < 3k-2$ and $k \geq 8$. We write $k = 4p + r,\ 1 \leq r \leq 4$. Then the values of n_2, n_3 and n_4 are determined by the following equations.*

$$n_2 = \begin{cases} 0, & n \leq 2k-p-2 \text{ or } n = 2k-p-1, r = 1, 2; \\ 1, & n = 2k-p, r = 1; \\ n-2k+p+2, & 2k-p-r+2 \leq n \leq 3k-p-2; \\ k, & 3k-p-1 \leq n < 3k-2. \end{cases} \tag{3.1}$$

$$n_3 = \begin{cases} 2n-3k+2, & n \leq 2k-p-2;\ \text{or } n = 2k-p-1, r = 1, 2; \\ k-2p, & n = 2k-p, r = 1; \\ k-2p-2, & 2k-p-r+2 \leq n \leq 3k-p-2; \\ 2n-5k+2, & 3k-p-1 \leq n < 3k-2. \end{cases} \tag{3.2}$$

$$n_4 = \begin{cases} 2k-n-2, & n \leq 2k-p-2;\ \text{or } n = 2k-p-1, r = 1, 2; \\ p-1, & n = 2k-p, r = 1; \\ p, & 2k-p-r+2 \leq n \leq 3k-p-2; \\ 3k-n-2, & 3k-p-1 \leq n < 3k-2. \end{cases} \tag{3.3}$$

Proof. From (2.1) we have

$$\begin{cases} n_3 = 2n - 3k - 2n_2 + 2 \\ n_4 = 2k + n_2 - n - 2. \end{cases} \tag{3.4}$$

Hence we have

$$2n_4 + 2 - n_3 = 7k + 4n_2 - 4n - 4. \tag{3.5}$$

It suffices to prove (3.1) since (3.2) and (3.3) can be obtained from (3.4) immediately.

From Lemma 2.7, we know that $n_4 \neq 0$, $e_{22} = 0$ and $n_2 \leq k$.

By Corollary 2.4(1) and (3.5), we have

$$e_{14} = 2n_4 + 2 - e_{34} - e_{24} \geq 2n_4 + 2 - n_3 - n_2 = 7k + 3n_2 - 4n - 4. \tag{3.6}$$

By Corollary 2.4(2) and (3.5), we have

$$e_{33} = n_3 - (2n_4 + 2) + e_{14} + e_{24} \geq -7k - 4n_2 + 4n + 4. \tag{3.7}$$

Now we are going to prove (3.1) according to the range of n which is divided into four cases as follows:

Case 1. $n \leq 2k - p - 2$, or $n = 2k - p - 1$ and $r = 1, 2$.

If $n \leq 2k - p - 2$, then by (3.6) we have

$$\begin{aligned} e_{14} &\geq 7k + 3n_2 - 4n - 4 \geq 7k + 3n_2 - 4(2k - p - 2) - 4 \\ &= 3n_2 + 4p + 4 - k = 3n_2 + 4 - r \geq 3n_2. \end{aligned}$$

If $n = 2k - p - 1 =$ and $r = 1, 2$, then

$$\begin{aligned} e_{14} &\geq 7k + 3n_2 - 4n - 4 = 7k + 3n_2 - 4(2k - p - 1) - 4 \\ &= 3n_2 + 4p - k = 3n_2 - r \geq 3n_2 - 2. \end{aligned}$$

From Lemma 2.5(2) we know that either $e_{14} = 0$ or $n_2 = 0$. Thus, $n_2 = 0$.

Case 2. $n = 2k - p$ and $r = 1$.

Suppose $n_2 = 0$. Then $e_{12} = 0$. From the first equality of (3.7), we have

$$e_{33} \geq -7k - 4n_2 + 4n + 4 = 4(2k - p) + 4 - 7k = 4 + r = 5.$$

By Lemma 2.5(3) and Lemma 2.6(1) we have $e_{14} = e_{13} = 0$. Combining with $e_{12} = 0$ we have $k = 0$, which is impossible. Hence $n_2 \neq 0$. By Lemma 2.5(2) we have $e_{14} = 0$.

From (3.6) we have

$$\begin{aligned} e_{14} &\geq 7k + 3n_2 - 4n - 4 = 7k + 3n_2 - 4(2k - p) - 4 \\ &= 3n_2 + 4p - k - 4 = 3n_2 - r - 4 = 3n_2 - 5. \end{aligned}$$

Hence $n_2 = 1$.

Case 3. $2k - p - r + 2 \leq n \leq 3k - p - 2$.

Suppose $n_2 \geq n - 2k + p + 3$. Then $n_2 \geq (2k - p - r + 2) - 2k + p + 3 = -r + 5 > 0$. Thus $e_{14} = 0$ by Lemma 2.5(2). By Corollary 2.4(1) and (3.5),

$$\begin{aligned} e_{24} &= 2n_4 + 2 - e_{14} - e_{34} = 2n_4 + 2 - e_{34} \geq 2n_4 + 2 - n_3 = 7k + 4n_2 - 4n - 4 \\ &\geq 7k + 4(n - 2k + p + 3) - 4n - 4 \geq -r + 8 \geq 4, \end{aligned}$$

which contradicts to Lemma 2.5(1). Therefore $n_2 \leq n - 2k + p + 2$.

Suppose $n_2 \leq n - 2k + p$. Then by (3.7)

$$e_{33} \geq -7k - 4(n - 2k + p) + 4n + 4 = r + 4 \geq 5.$$

Hence by Lemma 2.6(1) we have $e_{13} = 0$. On the other hand, from Corollary 2.8(2) we have $e_{13} = k - n_2 \geq k - (n - 2k + p) \geq 3k - (3k - p - 2) - p = 2$. It yields a contradiction. Therefore $n_2 = n - 2k + p + 1$ or $n_2 = n - 2k + p + 2$.

If $n_2 = n - 2k + p + 1$, then by (3.7) we have

$$e_{33} \geq -7k - 4(n - 2k + p + 1) + 4n + 4 = r \geq 1.$$

Thus $e_{14} = e_{24} = 0$ by Lemma 2.5(3).

Recall that $e_{22} = 0$ and $n_4 \neq 0$. By Corollary 2.3(3) we have

$$e_{23} = n_2 = n - 2k + p + 1 \geq (2k - p - r + 2) - 2k + p + 1 = 3 - r.$$

From (2.1) we have

$$\begin{aligned} e_{13} &= k - e_{12} - e_{14} \geq k - n_2 = k - (n - 2k + p + 1) \\ &\geq 3k - (3k - p - 2) - p - 1 = 1. \end{aligned}$$

Now we have $e_{13} \neq 0$ and $e_{33} + e_{23} \geq r + (3 - r) = 3$, which contradicts to Lemma 2.6(2). Therefore $n_2 = n - 2k + p + 2$.

Case 4. $3k - p - 1 \leq n < 3k - 2$. By (3.7) we have

$$e_{33} \geq -7k - 4n_2 + 4n + 4 > -7k - 4n_2 + 12k - 4p - 8 + 4 = 4(k - n_2) + r - 4.$$

If $n_2 < k$, then $e_{33} > 0$. By Lemma 2.5(3) we have $e_{14} = e_{24} = 0$. Thus by (2.1) we have $e_{13} = k - e_{12} \geq k - n_2 > 0$. By Corollary 2.3(3), we have

$$\begin{aligned} e_{23} &= n_2 = n - k - n_3 - n_4 > (3k - p - 2) - k - n_3 - n_4 \\ &= 2k - p - 2 - n_3 - n_4 \\ &= 2(4p + r) - p - 2 - (4p + r - 2n_4 - 2) - n_4 \\ &= 3p + n_4 + r \geq 5. \end{aligned}$$

This contradicts to Lemma 2.6(2). Therefore $n_2 = k$. $\square$

Next we will determine the values of e_{ij}, $i = 1, 2, 3, 4$ and $i < j \leq 4$. We have the following result.

Theorem 3.2. *Suppose $T \in \mathcal{T}_{n,k}$ is a maximal chemical tree. If $(3k - 2)/2 \leq n < 3k - 2$ and $k = 4p + r \geq 8$ $(1 \leq r \leq 4)$, then*

$$\begin{pmatrix} e_{12} \\ e_{13} \\ e_{14} \\ e_{22} \\ e_{23} \\ e_{24} \\ e_{33} \\ e_{34} \\ e_{44} \end{pmatrix} = \begin{pmatrix} n_2 \\ k - n_2 \\ 0 \\ 0 \\ n_2 \\ 0 \\ 2n_3 - k \\ k - n_3 \\ n_4 - 1 \end{pmatrix}, \quad \begin{pmatrix} n_2 \\ k - n_2 \\ 0 \\ 0 \\ n_2 - 4 + r \\ 4 - r \\ 0 \\ n_3 \\ n_4 - 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 2n_3 \\ k - 2n_3 \\ 0 \\ 0 \\ 0 \\ 0 \\ n_3 \\ n_4 - 1 \end{pmatrix} \tag{3.8}$$

corresponding to $n_3 \geq 2n_4 + 2$, $n_3 < 2n_4 + 2$ *and* $n_2 \neq 0$, $n_3 < 2n_4 + 2$ *and* $n_2 = 0$, *respectively. Hence we have*

$$R_{\max}(T) = \begin{cases} \dfrac{n_2}{\sqrt{2}} + \dfrac{k-n_2}{\sqrt{3}} + \dfrac{n_2}{\sqrt{6}} + \dfrac{2n_3-k}{\sqrt{9}} + \dfrac{k-n_3}{\sqrt{12}} + \dfrac{n_4-1}{\sqrt{16}}, & n_3 \geq 2n_4+2; \\ \dfrac{n_2}{\sqrt{2}} + \dfrac{k-n_2}{\sqrt{3}} + \dfrac{n_2-4+r}{\sqrt{6}} + \dfrac{4-r}{\sqrt{8}} + \dfrac{n_3}{\sqrt{12}} + \dfrac{n_4-1}{\sqrt{16}}, & n_3 < 2n_4+2, n_2 \neq 0; \\ \dfrac{2n_3}{\sqrt{3}} + \dfrac{k-2n_3}{\sqrt{4}} + \dfrac{n_3}{\sqrt{12}} + \dfrac{n_4-1}{\sqrt{16}}, & n_3 < 2n_4+2, n_2 = 0. \end{cases}$$

Proof. First, we have $n_4 \neq 0$ by Lemma 2.7. Then $e_{22} = 0$ by Lemma 2.5(4). Thus $e_{12} = n_2$. By Corollary 2.3(2), $e_{44} = n_4 - 1$.

For $n_3 \geq 2n_4 + 2$, $e_{13}, e_{23}, e_{33}, e_{14}, e_{24}$, and e_{34} are determined by Corollary 2.8. So we assume that $n_3 < 2n_4 + 2$. By the equality part of (3.7) we have $e_{33} = n_3 - (2n_4 + 2) + e_{14} + e_{24} < e_{14} + e_{24}$. From Lemma 2.5(3) we know that either $e_{14} = e_{24} = 0$ or $e_{33} = 0$. Thus we have $e_{33} = 0$. Hence from Corollary 2.3(4), we get $e_{34} = n_3 - e_{33} = n_3$. Thus, the values of e_{13}, e_{23}, e_{14} and e_{24} remain to be determined.

By (3.1) and (3.5), we have

$$n_3 - (2n_4+2) = \begin{cases} 4n-7k+4, & n \leq 2k-p-2;\ \text{or}\ n = 2k-p-1, r = 1,2; \\ 1, & n = 2k-p, r = 1; \\ r-4, & 2k-p-r+2 \leq n \leq 3k-p-2; \\ 4n-11k+4, & 3k-p-1 \leq n < 3k-2. \end{cases} \tag{3.9}$$

Case 1. $n_3 < 2n_4 + 2$ and $n_2 \neq 0$.

Since $n_2 \neq 0$, $e_{14} = 0$ by Lemma 2.5(2). From (3.9) and (3.1), it is easy to see that this case is equivalent to $2k - p - r + 2 \leq n \leq 3k - p - 2$ and $r \neq 4$. By Corollary 2.4(2), we have $e_{24} = 2n_4 + 2 - n_3 = 4 - r$. From (2.1) we have $e_{13} = k - e_{12} - e_{14} = k - n_2$. Finally, by Corollary 2.3(3) we have $e_{23} = n_2 - e_{24} = n_2 - 4 + r$.

Case 2. $n_3 < 2n_4 + 2$ and $n_2 = 0$.

In this case, it is clear that $e_{12} = e_{23} = e_{24} = 0$. Furthermore, $e_{14} = (2n_4 + 2) - n_3$ by Corollary 2.4(2). Since $k = n_3 + 2n_4 + 2$ and $k = e_{12} + e_{13} + e_{14}$ from (2.1), $e_{14} = k - 2n_3$ and $e_{13} = 2n_3$.

Thus we have (3.8). By substituting the results of (3.8) into (1.1) we have the theorem. □

By properties stated in Section 2, it is not difficult to get that

$$(e_{12}, e_{13}, e_{14}, e_{22}, e_{23}, e_{24}, e_{33}, e_{34}, e_{44}) = (k, 0, 0, n-3k+2, k, 0, k-3, 0, 0),$$

for $n \geq 3k - 2$. Hence we obtain the following theorem.

Theorem 3.3 ([3,6,13]). *If* $n \geq 3k - 2$, *then*

$$R_{\max}(\mathcal{T}_{n,k}) = \frac{n}{2} + \frac{(3\sqrt{2}+\sqrt{6}-7)k}{6}.$$

4. Constructions of some maximum trees

For convenience, a chemical tree is called a 4-*regular tree* if $V(T) = V_1(T) \cup V_4(T)$.

Suppose $T \in \mathcal{T}_{n,k}$ is a maximal chemical tree. If $n \geq 3k - 2$, then the construction of T is given in [6,13]. If $n < 3k - 2$ and $k \geq 8$, then a maximal chemical tree T can be constructed by the following steps. Note that maximal chemical tree of order n with k pendants is not unique.

First, determine the values of n_2, n_3 and n_4 by applying (3.1)–(3.3). Then construct a 4-regular tree T_1 such that $|V_4(T_1)| = n_4$.

(1) If $n_3 < 2n_4 + 2$ and $n_2 = 0$, then T can be obtained from T_1 by attaching two edges to each of n_3 pendants of T_1. Then T satisfies

$$(e_{12}, e_{13}, e_{14}, e_{22}, e_{23}, e_{24}, e_{33}, e_{34}, e_{44}) = (0, 2n_3, k-2n_3, 0, 0, 0, 0, n_3, n_4-1).$$

(2) If $n_3 < 2n_4+2$ and $n_2 \neq 0$, then from the proof of Case 1 of Theorem 3.2 we have $2n_4+2-n_3 = 4-r$ and $n_2 \geq 4-r$. Let T_2 be the tree obtained from T_1 by choosing n_3 pendants of T_1 and attaching two edges to each of them and attaching one edge to each of remaining $4 - r$ pendants. And then T can be obtained from T_2 by attaching one edge to each of $n_2 - 4 + r$ 3-degree pendant edges, respectively. Then T satisfies

$$(e_{12}, e_{13}, e_{14}, e_{22}, e_{23}, e_{24}, e_{33}, e_{34}, e_{44}) = (n_2, k-n_2, 0, 0, n_2-4+r, 4-r, 0, n_3, n_4-1).$$

(3) If $n_3 \geq 2n_4 + 2$, then T_2 can be obtained from T_1 by attaching two edges to each pendant of T_1. Let T_3 be obtained from T_2 by attaching two edges to each of its $n_3 - 2n_4 - 2$ pendants. And then let T be obtained from T_3 by attaching one edge to each of its n_2 pendants. Then T satisfies

$$(e_{12}, e_{13}, e_{14}, e_{22}, e_{23}, e_{24}, e_{33}, e_{34}, e_{44}) = (n_2, k-n_2, 0, 0, n_2, 0, n_3-(2n_4+2), 2n_4+2, n_4-1).$$

According to Theorems 3.2 and 3.3, the trees T constructed above are maximal chemical trees. Examples for $k = 4p+r = 9 (p = 2, r = 1)$, $13 = \lceil \frac{3k-2}{2} \rceil \leq n \leq 3k - 2 = 25$ are shown in Fig. 5.

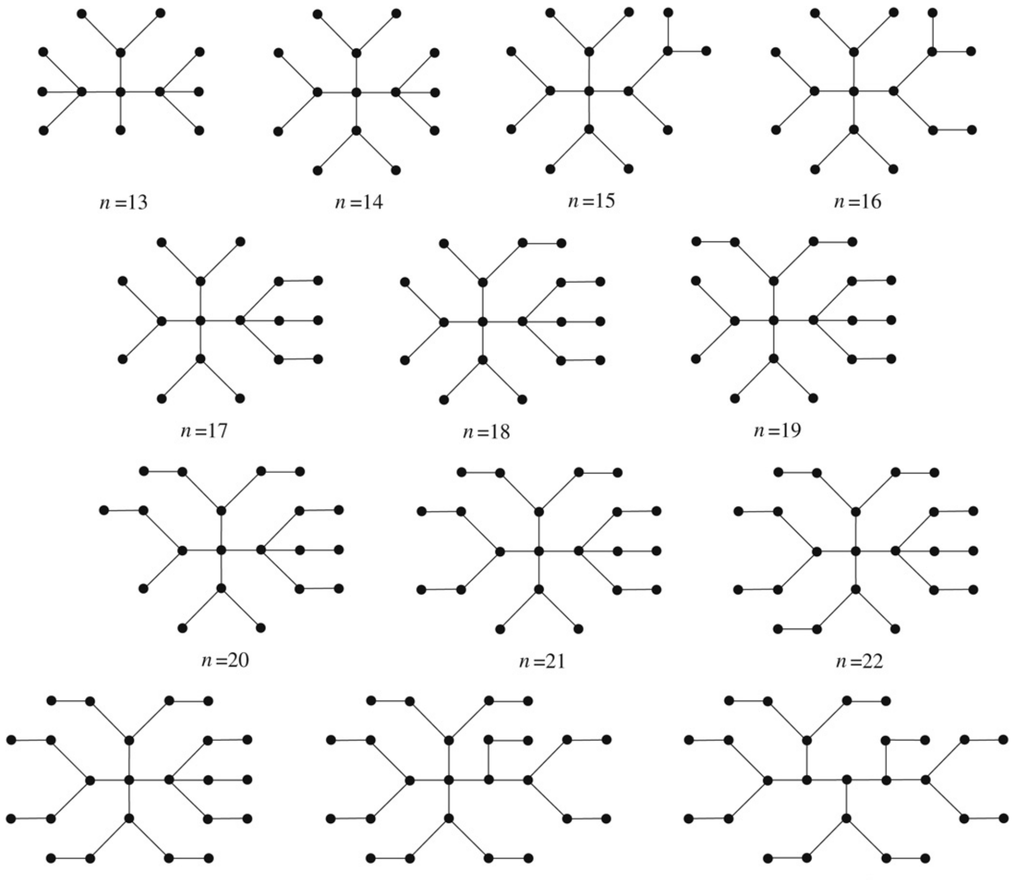

Fig. 5. Examples of maximal chemical trees for $13 \leq n \leq 25$ and $k = 9$.

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